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Pseudopotential dependence of superconducting state parameters of Bi based binary alloys

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Abstract : The pseudopotential formalism for binary alloy superconductors due to Allen and Dynes and Khan *et al* has been applied for the study of dependence of the superconducting state parameters like electron phonon coupling strength λ, transition temperature T_c, isotope effect exponent α and the interaction strength N_0V on the pseudopotential form factors. Six pseudopotentials in conjunction with RPA form of dielectric screening have been employed for the calculation of the above mentioned parameters for a number of Bi-based alloys. On comparing the calculated T_c values with experimental data available in literature, it has been observed that the linear potential provides the best results for $Bi_{1-c}In_c$ and $Bi_{1-c}Sb_c$ alloys whereas the linearised screened pseudopotential yields results in good agreement for $Bi_{1-c}In_c$, $Bi_{1-c}Tl_c$ and $Bi_{1-c}Pb_c$ alloys. The values of α and N_0V for these alloys have been calculated by using the best pseudopotentials mentioned above.

Keywords : Pseudopotential, binary alloys, superconducting state

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The discovery of high temperature superconductivity [1,2] in metallic oxides like $La_{2-x}(Sr, Ba)_xCuO_4$, $YBa_2Cu_3O_{7-\delta}$ *etc* has created renewed interest in the alloys of metallic superconductors. The BCS-Eliashberg-McMillan's formalism [3–5] for metallic superconductors was extended by Allen and Dynes [6] for its application to the binary alloys. Khan *et al* [7] reexamined the formalism and applied it to a number of In-based alloys. The results obtained by them were in good agreement with available experimental data.

The selections of appropriate forms of the pseudopotential and the dielectric screening function are the essential ingredients of a successful pseudopotential analysis of metallic alloys. The former can be accomplished by carrying out the study of the dependence of superconducting state parameters of the alloy superconductors on the pseudopotential form factors. The present authors investigated earlier [8] the dependence of superconducting state parameters on dielectric screening function and it was found that the Random Phase Approximation (RPA) form [9] of the dielectric screening is the best for explaining the

superconducting behaviour of the In-based alloys. As such, this form of the screening was considered suitable for Bi-based alloys also.

In the present work, superconducting state parameters λ, μ^* and T_c are determined by employing six different forms of the pseudopotential form factors on the basis of McMillan's formalism [4,5] for the alloys under consideration with Bi as host and In, Tl, Sb and Pb as impurities at different concentrations. These results have been compared with experimental data. The values of the isotope effect exponent α and the interaction strength N_0V have also been worked out by employing the pseudopotentials which provide T_c values in the best agreement with the experimental data. The dependence of α and N_0V on concentration of the impurity have been shown pictorially in the form of curves (Figures 1 and 2).

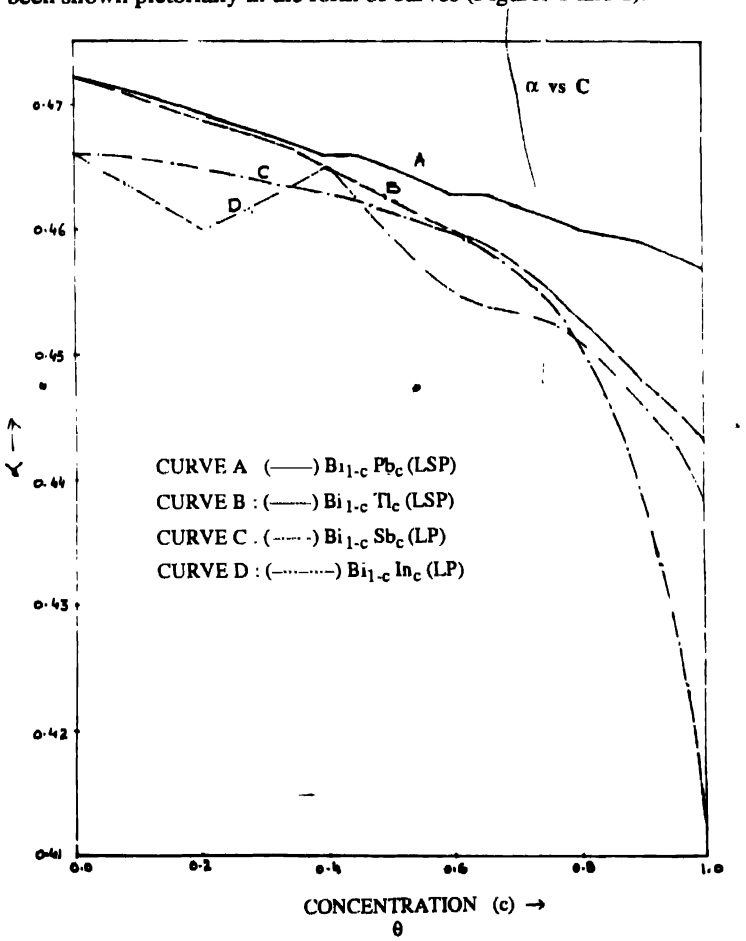

Figure 1. The variation of isotope effect exponent α with concentration (c) of impurity in host Bismuth.

The expressions employed for the evaluation of the superconducting state parameters are given by [8]

$$\lambda_{AB} = \frac{^{12}(m_b)_{AB} Z_{AB}}{M_{AB} < w >^2_{AB}} \int_0^1 x^3 \left|V_{AB}(x)\right|^2 dx, \tag{1}$$

$$\mu^*_{AB} = \frac{\dfrac{(m^*)_{AB}}{\pi(k_F)_{AB}} \displaystyle\int_0^1 \frac{dx}{x\varepsilon(x)}}{1 + \dfrac{(m^*)_{AB}}{\pi(k_F)_{AB}} \ln\left(\dfrac{(k_F^2)_{AB}}{20(\theta_D)_{AB}}\right) \displaystyle\int_0^1 \frac{dx}{x\varepsilon(x)}}, \tag{2}$$

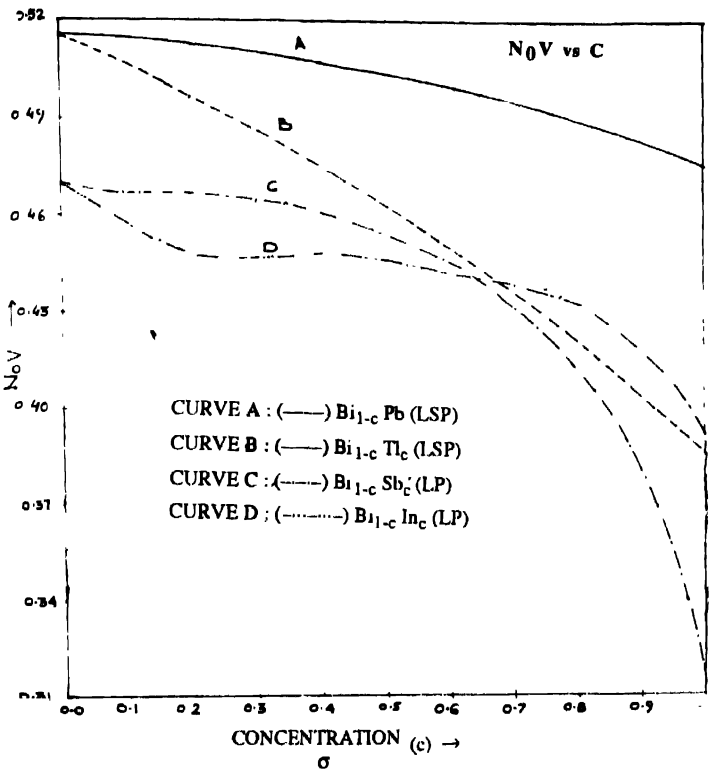

Figure 2. The variation of interaction strength N_0V with concentration (c) of impurity in host Bismuth.

$$(T_c)_{AB} = \frac{(\theta_D)_{AB}}{1.45} \exp\left[\frac{1.04\ (1 + \lambda_{AB})}{\lambda_{AB} - \mu^*_{AB}\ (1 + 0.62\ \lambda_{AB})}\right], \tag{3}$$

$$(\alpha)_{AB} = \frac{1}{2}\left[1 - \left(\mu^*_{AB} \ln \frac{(\theta_D)_{AB}}{1.45\ (T_c)_{AB}}\right)^2 \cdot \frac{1 + 0.62\lambda_{AB}}{1.04\ (1 + \lambda_{AB})}\right], \tag{4}$$

and

$$(N_0V)_{AB} = \frac{\lambda_{AB} - \mu^*_{AB}}{1 + (10/11)\ \lambda_{AB}}, \tag{5}$$

Table 1. Transition temperature T_c(°K) of Bi-based alloys

Alloy	Conc.	Pseudopotentials employed in present calculation						Experimental result
		HA	LP	ASC	LSP	VS	HP	
$Bi_{1-c}In_c$	0 0	09.463	6 545	11.259	8 192	11.680	09 226	6.1
	0.667	03.588	5.111	00.795	5 553	04 374	10 226	5 6
	0.78	02.520	4 866	00.206	4 798	03.132	11.143	4.53
	0 95	00 993	3 994	00.002	3.249	01.351	11 593	4 27
	0.994	00.653	3.600	1.2×10^{-4}	2 731	00 937	11 457	3 495
	1.0	00.595	3.539	7.6×10^{-5}	2.656	00 883	11.427	3.40
$Bi_{1-c}Tl_c$	0.0	09.463	6.545	11.259	8.192	11.680	09.226	6 1
	0 333	05.959	5.066	4.199	6.154	06 420	05 063	6.4
	0.9	01.785	4 496	0 0229	3 225	00 974	06 286	2 3
	1.0	01.285	4.356	0.0028	2 748	00 532	06 538	2.36
$Bi_{1-c}Sb_c$	0.0	09 463	6.545	11.259	08.192	11.680	09.226	6.1
	0.03	09.561	6.604	11.080	08 171	11.877	09.334	7.2
	0.2	10.136	6 938	10.045	08.012	13 044	09 978	6.3
	0.6	11.307	7.401	8 114	07 022	16.029	11.470	6.3
	1.0	07.324	3.354	4.793	01.888	14.933	08.096	3.55–3.4
$Bi_{1-c}Pb_c$	0.0	09.463	6.545	11.259	08.192	11.680	09 226	6.1
	0.45	05.792	0.188	04.116	06 884	05.826	04.112	7.0
	0.65	04.429	6.01×10^{-3}	02.015	06 318	04.331	04.988	8.95
	0.7	04.113	1.87×10^{-3}	01.613	06.175	04.059	05.272	8.45
	0.8	03 498	1.12×10^{-4}	00.962	05.885	03 619	05 840	7.95
	0.9	02.864	3.06×10^{-6}	00 507	05 588	03.301	06 360	7.65
	1.0	02.689	2.94×10^{-8}	00.224	05 284	03.081	06.801	7.2

where AB refers to alloys $A_{1-c}B_c$ and M and Z are ionic mass and valency of metal respectively. $V_{AB}(x)$ in eq. (1) represents screened pseudopotential form factors which are given by

$$V_{AB}(x) = \frac{V^b_{AB}(x)}{\epsilon(x)}, \tag{6}$$

where $V^b_{AB}(x)$ are the bare electron ion form factors for the alloy and $\epsilon(x)$ is the dielectric screening function, for which R.P.A. form [9] has been employed. The different forms of the pseudopotentials used in this work are :

(1) Heine-Abarenkov potential (V_{HA}) [10]; (2) Linear potential (V_{LP}) [11]; (3) Aschroft's potential (V_{ASC}) [12]; (4) Linearised screened pseudopotential (V_{LSP}) [13]; (5) Veljkovic and Slavic potential (V_{VS}) [14]; (6) Harrison potential (V_{HP}) [15]. Vegard's rule has been employed for obtaining the relevant pseudopotentials for the alloys under consideration.

The input parameters required in this work are obtained for the alloys under consideration from the metallic data by the use of Vegard's rule except for θ_D which is obtained from the Grimvall's relation [16]. Similarly, the most representative root mean square frequency $<w^2>^{1/2}$ for the alloy is obtained from the relevant metallic frequencies by

$$\frac{1}{\langle w^2\rangle^{1/2}_{AB}} = \frac{1-c}{\langle w^2\rangle^{1/2}_{A}} + \frac{c}{\langle w^2\rangle^{1/2}_{B}}. \tag{7}$$

The values of the input parameters *i.e.*, band mass (m_b), effective mass (m^*), Debye temperature (θ_D), Fermi radius (k_F) and the most representative phonon frequencies for the longitudinal and transverse branches (w_L and w_T) have been taken from ref [11], except for Bi and Sb. The values of m_b, m^* and k_F for Bi as well as the value of k_F for Sb and the atomic volume for all metals have been taken from ref [17]. The values of m_b and m^* for Sb have been taken equal to one as the relevant date is not available in literature. The values of θ_D for both the semimetals have been taken from ref [18] and values of $<w^2>^{1/2}$ have been calculated by using the empirical relation $<w^2>^{1/2} = 0.69\ \theta_D$ due to Butler [19]. The potential parameters have been taken from relevant references [7,11,13,17 and 20] for the metallic phases, except for Bi and Sb for which their values are obtained by fitting the pseudopotential form factors.

Table 1 contains the presently calculated values of transition temperature T_c alongwith the experimental data [6,21]. It may be observed that the linear potential provides the best results for $Bi_{1-c}In_c$ and $Bi_{1-c}Sb_c$ alloys whereas the linearised screened pseudopotential yields results in good agreement for $Bi_{1-c}In_c$, $Bi_{1-c}Tl_c$ and $Bi_{1-c}Pb_c$ alloys. These values also show good agreement with the other theoretical results [22 and 23].

The values of isotope effect exponent α and the interaction strength N_0V for these alloys have been calculated by using the pseudopotentials which provide best match with

experimental T_c, as discussed above. These results have been shown in Figures 1 and 2 respectively. From these figures, it may be observed that the α and N_0V values show small changes with concentration (c) for $Bi_{1-c}Pb_c$ alloys whereas the variation is considerable for the case of $Bi_{1-c}Sb_c$ alloys. For other alloys the variation has been found to be moderate. From curve D in Figure 1, we notice two peak-like structures at concentrations $c = 0.4$ and 0.75 approximately for $Bi_{1-c}In_c$ alloys. Similar structures though less prominent, are also observed for this system from curve D in Figure 2. These structures suggests stoichiometrically favourable phases providing stronger coupling at these concentrations.

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